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14. ABSTRACT
This is the first annual report of a project that uses locally-developed TOMBO (TOhoku Mixed Basis Orbitals ab-initio program) to study electron transport properties of materials. TOMBO employs mixed basis, composed of plane wave basis sets and atomic basis sets.

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Part 1. Calculation of electron transport property by TOMBO

INTRODUCTION

The interest in the electron transport phenomena through organic molecule and nano systems has been triggered recently. Different experimental methods have been achieved to observe and measure the current/spin current in order to develop next generation electronic devices. Some prospective candidates, such as benzene polymer and carbon nano tube, have been proposed to realize this interesting property.

To facilitate the understanding of these phenomena and to predict new candidates, different theoretical methods have been applied. With the development of computational methods and resources since these years, it becomes possible to study these problems based on the first-principles calculation within density functional theory.

TOMBO (TOhoku Mixed Basis Orbitals *ab-initio* program) is developed by Kawazoe Laboratory. Mixed basis, composed of plane wave basis sets and atomic basis sets, is used in TOMBO. Now, we are trying to use TOMBO to study the electron transport properties.

METHODOLOGY

Direct application of TOMBO to the numerical calculation of electron transport is impossible, because in the calculation the whole system is divided into three different parts and they should be treated separately. Therefore, the maximum localized Wannier function (MLWF) has to be used. MLWF can achieve the unitary transformation with the most localized spread.

With the help of MLWF, it becomes possible to transform our basis sets from reciprocal space to the real space and the algorithm of our calculation works as follows,

1) The surface Green functions of two electrodes are computed.
2) The whole system is calculated and the interaction between the nano system and the both electrodes is extracted by using MLWF.
3) The self-energy terms representing two electrodes are added into Hamiltonian.
4) The non-equilibrium Green's function (NEGF) is used to calculate the new density matrix, and from this new density matrix, we can get a new Hamiltonian and the algorithm is solved self-consistently until it is converged.

RESULTS

By now, the extraction of density matrix and the Hamiltonian from TOMBO is finished and invoking Wannier90 library solves MLWF. We are developing the interface between TOMBO and MLWF. With this interface, MLWF can be used seamlessly and the plane wave basis sets can be converted into real space basis sets.

Part 2. Calculation of thermal transport property by TOMBO

INTRODUCTION

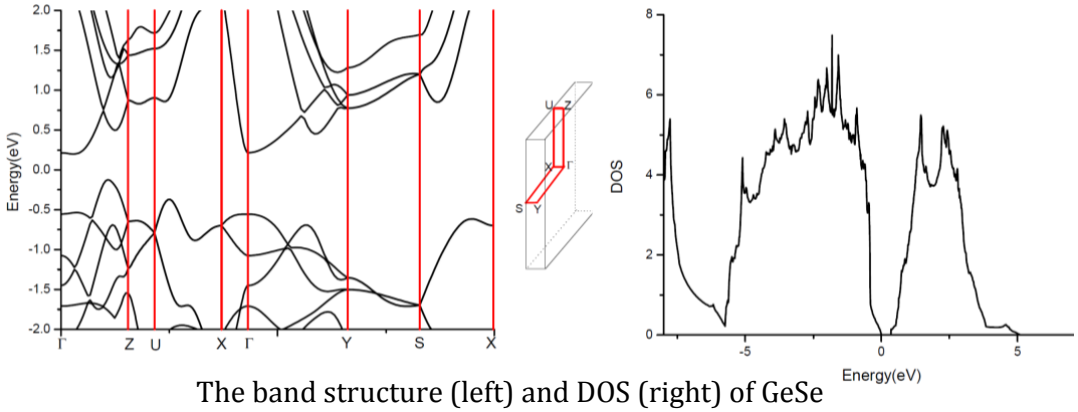
Thermoelectric materials are used in solid-state devices which convert wasted heat into electricity. The efficiency of the device depends on both the thermoelectric materials used and on the system design. In this work, we plan to investigate the thermal properties of GeSe as a novel efficient thermoelectric material, using first-principles density-functional calculations. The calculations proceed in several stages: first the electronic structure of the relaxed structure will be computed, next, from force calculations in a large supercell, we extract the harmonic and anharmonic force constants, and finally from the latter we calculate the phonon dispersion and lifetimes which will be used in the calculation of the lattice thermal conductivity using the relaxation time approximation. These studies can later be extended to other similar structures such as GeTe and SnSe, or their alloys.

METHODOLOGY

We use the VASP package to perform the first-principles calculations. The PBEsol exchange-correlation functional is used to optimize the lattice parameters. GeSe is an orthorhombic crystal with space group Pnma. In this case, 4x10x8 k-points are used with a cutoff energy of 500.0 eV.

RESULTS

The optimum lattice parameters are 10.846 x 3.905 x 4.299 Angs. This is within 2% of the experimental values of 10.83 x 3.83 x 4.39 Angs. The electronic band structure and density of states (DOS) are potted in the following figures.



The band structure (left) and DOS (right) of GeSe

We can note that GeSe is an indirect gap semiconductor of bandgap 0.33 eV in the Γ-Z direction. The available experimental value for the optical DIRECT GAP is 1.1 eV. In our calculations, the direct gap is 0.76 eV at the zone center, consistent with the expected underestimation in all LDA or GGA calculations.

For the next trimester, we will perform the supercell calculations of the forces, from which force constants will be extracted, and tested for reliability. The following trimester, these force constants will be used in the calculation of phonon dispersion, Gruneisen parameters and lifetimes, as well as the thermal conductivity. If the calculations are successful, we will then proceed to calculate other similar compounds such as GeS, GeTe…